10,11-Dihydro-5H-dibenz(b,f)azepin-5-amine 7458-07-3 | DTXSID00225559

Model Performance

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)		
Q2	RMSE	R2	RMSE	R2	RMSE	
0.95	0.69	0.95	0.65	0.96	0.68	

Model Results

Predicted value: 9.22

Global applicability domain: Inside

Local applicability domain index: 7.38e-01

Confidence level: 3.65e-01

Nearest Neighbors from the Training Set

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Phenacetin Measured: 9.59 Predicted: 9.23 Image not found

Diphenylamine Measured: 7.64 Predicted: 8.73 Image not found

1-Hexadecanol Measured: 9.90 Predicted: 9.79

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Methylparaben Measured: 8.57 Predicted: 7.06 Image not found

1-Octadecanol Measured: 10.9 Predicted: 10.5